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COMPUTRATIONAL METHODS FOR FLOW PROBLEMS - PARALLEL ALGORITHMS, FLOW CONTORL, AND NOVEL APPROACHES

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A review of the research that has been carried out under the sponsorship of Air Force Office of Scientific Research grant number AFOSR-90-0179 is given. Details are given about two research programs, namely flow control and superconductivity. In both instances we have modeled realistic physical problems, we have performed rigorous analyses on the mathematical models, we have developed approximation schemes which we have also analyzed, and we have written computer codes implementing our computational method. In both instances, we were the first to carry out such a comprehensive research program, and in so doing, have developed robust and useful algorithms that may be applied to practical problems. In connection with our research in flow optimization, we have also embarked on a joint research program with personnel at the AEDC facility in Tullahoma, Tennessee. We also briefly discuss other accomplishments related to this grant, including other research projects, invited talks, journal articles, etc.

I - REVIEW OF RESEARCH ACCOMPLISHMENTS UNDER GRANT NUMBER AFOSR-90-0179

We begin by reviewing some of the research that has been completed and that has been supported by AFOSR under Grant Number AFOSR-90-0179. For the sake of brevity, we will not go into great detail in the following discussion; further information concerning these topics can be gained from the appropriate references listed in §III. Also, again for the sake of brevity, we will only discuss two of the areas of research with which we have been concerned. Other research projects are briefly discussed in §II.

1. Numerical Solution of Flow Control Problems

Over the past few years we have undertaken a comprehensive research program addressing various issues connected with flow control and optimization problems. Our efforts in this direction have focused on

- building mathematical models of the physical problems, invoking a minimum of assumptions about the physical phenomena;
- rigorously analyzing the mathematical models, for example, to study the existence and regularity of solutions, to verify the existence of Lagrange multipliers to enforce constraints, and to derive necessary conditions that optimal controls must satisfy;
- constructing and analyzing discretization methods for determining approximate solutions of the optimal control and optimization problems, including a rigorous derivation of error estimates; and
- developing computer codes implementing our discretization algorithms, first for the purpose of showing the efficacy of these methods, and ultimately, to solve problems of practical interest.

Our success in carrying out the program is evidenced in various ways. We have published, or have had accepted, numerous articles in top-of-the-line journals; we have been asked to write chapters for books; we have been invited to lecture at many international conferences both of the mathematical and engineering persuasions; we were asked to organize and give the main talk at a workshop on flow control held in November, 1992 at the Institute for Mathematics and its Applications in Minnesota; and, perhaps most important, our ideas and algorithms are been used and implemented by engineers interested in flow control and optimization problems. Details concerning the papers, invited talks, and the Minnesota workshop may be found in §III; a discussion of a setting wherein our ideas are being implemented is discussed in §1.1.

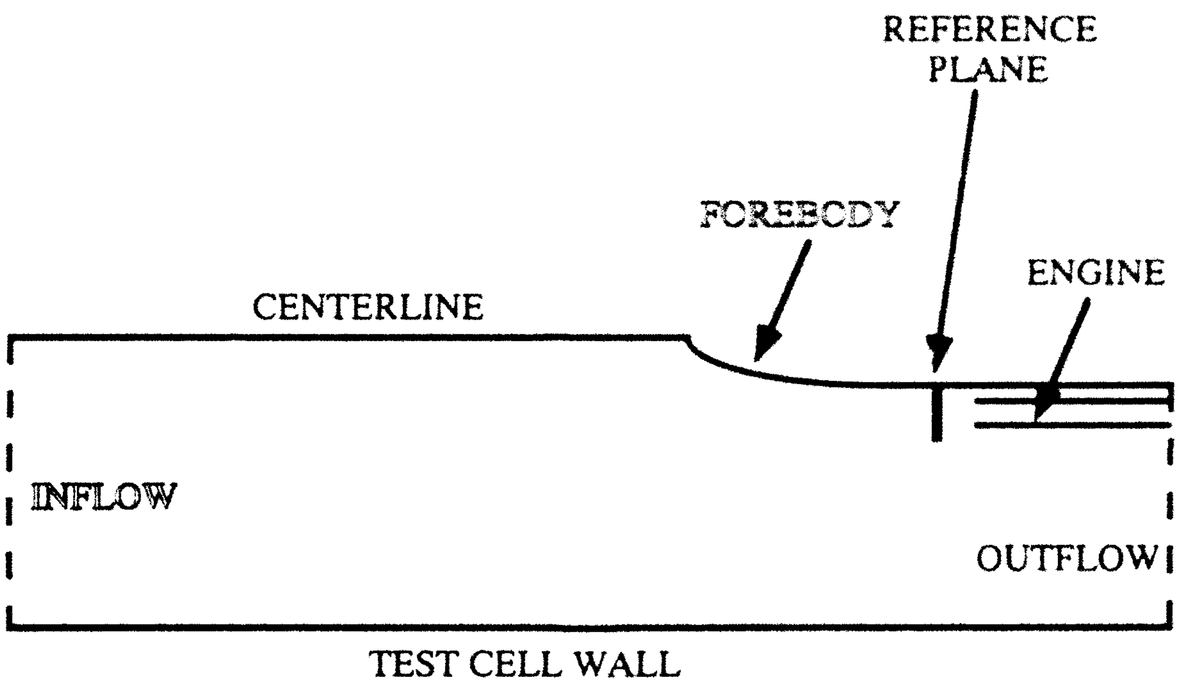
Our work on flow control deals with two different classes of methods of solution. In §1.1 we discuss our work on methods that use sensitivities within an optimization algorithm, while in §1.2 we deal with the adjoint, or co-state, or Lagrange multiplier approach.

1.1. *Design of the AEDC free-jet test facility*

An example of our efforts in using sensitivities in connection with flow control problems is the work we are doing in collaboration with engineers at the AEDC facility in Tullahoma, Tennessee. Our collaborators in this project include John Burns, Gene Cliff, and Jeff Borggard of Virginia Tech.

and Karl Kneile and Donald Todd of AEDC.

One of the primary missions of the AEDC facility is to test aircraft engines. Indeed, within the United States, they have the unique capability of testing full-size engines within the controlled environment of a wind tunnel. Ideally, one would like to have the flow entering the engine in the test facility to be exactly the same as that entering the engine if it were attached to an aircraft in flight. Thus, referring to the sketch in the figure, we would like the flow at a reference plane ahead of the engine in the test facility to be the same as that in a similarly situated plane ahead of the engine in flight. In order to match the flight conditions at the reference plane (the test facility is not large enough to accommodate the whole aircraft) one is free to choose the forebody shape and certain inflow parameters such as the total pressure and Mach number; see the figure.



Thus the optimization problem is easily stated: determine the inflow parameters and the forebody shape that minimizes the difference between the flow at the reference plane in the test facility and that in flight.

In order to explain our ideas in connection with this problem, we introduce some notation. The mathematical structure of our problem is similar to that of any optimization or control problem. First we have certain *state variables*, i.e., variables that serve to describe the state of the system. In our context these are given by the pressure p, the internal energy e, the density ρ, and the momentum field $\rho\mathbf{u}$, where $\mathbf{u}$ denotes the velocity. We collectively denote the state variables by ϕ. Next, we have control variables or *design parameters* which we collectively denote by g. In our context these include certain inflow conditions such as the total pressure and Mach number, as well as a finite set of parameters that determine the shape of the forebody. (Typically, the forebody is defined as a combination of Bezier curves that are determined by a finite set of parameters.) The next ingredient is an objective or *cost functional* $\mathcal{J}$ that in general depends on the state and may also depend on

the controls. In our case we can use

$$\mathcal{J}(\mathbf{u}) = \frac{1}{2}\int_{\Gamma_{RP}} |\mathbf{u} - \mathbf{U}_f|^2 \, d\Gamma \qquad (1)$$

where Γ_{RP} denotes the reference plane and $\mathbf{U}_f$ denotes the velocity field at the reference plane in flight. (The latter is obtained through experimental measurements.) The final ingredients are *constraints* which in our context we denote by $F(\phi, g) = 0$. These are merely the flow equations, or in a practical setting, discretized versions of the flow equations. Then, the problem in hand is the following *minimization problem*: find controls g and states ϕ such that $\mathcal{J}(\mathbf{u})$ is minimized, subject to $F(\phi, g) = 0$.

The approach used at AEDC for solving this optimization problem relies on the *Gauss-Newton* method:

Start with an initial guess g_0 for the design parameters.

For $k = 0, 1, 2, \ldots$,

1. use the discretized flow equations to find a state ϕ_k such that $F(\phi_k, g_k) = 0$;
2. compute the sensitivities $(\partial\phi/\partial g)|_{g_k}$
3. solve for the increment δ from

$$A\left(\frac{\partial\phi}{\partial g}\Big|_{g_k}, \frac{\partial\phi}{\partial g}\Big|_{g_k}\right)\delta = B\left(r|_{g_k}, \frac{\partial\phi}{\partial g}\Big|_{g_k}\right),$$

where $A(\cdot,\cdot)$ and $B(\cdot,\cdot)$ are appropriately defined bilinear forms and r denotes an appropriate residual.

4. Set $g_{k+1} = g_k + \delta$

The iteration is terminated whenever $|\delta|$, or perhaps $|\mathcal{J}(\mathbf{u}_k) - \mathcal{J}(\mathbf{u}_{k-1})|$, is smaller than some prescribed tolerance.

Two key observations concerning the above algorithm are that Step 1, the state calculation, has been carried out using PARC-codes developed at AEDC and that for Step 2, the calculation of the sensitivities, finite difference approximations

$$\frac{\partial\phi}{\partial g}\Big|_{g_k} \approx \frac{\phi(g_k) - \phi(\tilde{g})}{g_k - \tilde{g}} \qquad (2)$$

are used, where $\tilde{g}$ is some value close to g_k, and $\phi(\tilde{g})$ satisfies the constraint equations $F(\tilde{\phi}, \tilde{g}) = 0$. Thus, using (2), Steps 1 and 2 require multiple state calculations; indeed, one needs $N + 1$ state calculations, where N denotes the total number of design parameters. The necessity of multiple state computations make this approach prohibitively expensive, especially in three-dimensions.

Our first task was to make the calculation of Step 2 more efficient. We were constrained, for practical purposes, to use existing PARC-codes, or small variations of these. In this context, we suggested that the sensitivities should be computed directly as solutions of the state equations $F(\phi, g) = 0$ differentiated with respect to the design parameter, i.e.,

$$\left(\frac{\partial F}{\partial\phi}\Big|_{(\phi_k, g_k)}\right)\frac{\partial\phi}{\partial g}\Big|_{g_k} = -\frac{\partial F}{\partial g}\Big|_{(\phi_k, g_k)}. \qquad (3)$$

Note that $(\partial F/\partial\phi)|_{(\phi_k, g_k)}$ and $(\partial F/\partial g)|_{(\phi_k, g_k)}$ depend only on g_k and ϕ_k, so that they may be evaluated after Step 1. Then, one may solve the linear system (3) for the sensitivities $(\partial\phi/\partial g)|_{g_k}$.

We have determined how to compute the sensitivities within the PARC environment, and variants of a 2-D PARC code have been developed both at Virginia Tech and AEDC which in fact compute the sensitivities. Currently these codes have been run for the inflow and forebody design parameters. Results are very encouraging, e.g., savings of factors of 5 to 10 over the use of the difference approximation (2) have been demonstrated.

1.2. *Analysis and approximation of adjoint methods for flow control*

As was mentioned above, the structure of a flow control or optimization problem involves *objectives* that express why one wants to control the flow. Such goals are usually expressed in terms of the minimization of a *cost functional*. Also, we have *constraints* that determine what kind of flow one is interested in. The nature of the flow is expressed in terms of a specific set of flow equations, e.g., Euler, Navier-Stokes, stationary, time dependent, incompressible, compressible, etc. Finally, one has available *control mechanisms* or *design parameters* that are to be used to meet the objective. Controls are expressed in terms of unknown data in the problem specification.

In our own work on adjoint methods, we have considered a large variety of objectives and control mechanisms in the context of incompressible viscous flows. We have rigorously analyzed these methods with regard to the existence and regularity of optimal solutions and the existence of Lagrange multipliers, we have derived optimality systems that determine optimal controls and states, we have defined and analyzed finite element algorithms, and we have developed codes that implement the algorithms.

Among the objectives that we have treated are the following; this list is not exhaustive, but is merely representative. First, we have *flow tracking* wherein one wishes the velocity field to be as close as possible to a prescribed field. If $\mathbf{u}$ and $\mathbf{U}_d$ denote the velocity field and a prescribed velocity field, respectively, then we want to control the flow so that $\mathbf{u}$ is "close" to $\mathbf{U}_d$. For example, one can minimize the functional

$$\mathcal{J}_1(\mathbf{u}) = \frac{1}{4}\int_\Omega |\mathbf{u} - \mathbf{U}_d|^4 \, d\Omega$$

where Ω denotes the flow domain. A second objective we have treated is *viscous drag minimization*. This can be accomplished by minimizing the integral of the dissipation function, i.e.,

$$\mathcal{J}_2(\mathbf{u}) = \frac{\mu}{2}\int_\Omega |(\nabla\mathbf{u}) + (\nabla\mathbf{u})^t|^2 \, d\Omega\,,$$

where μ denotes the viscosity coefficient. Another important objective is the *avoidance of hot spots*, i.e., places where temperature peaks occur, along bounding surfaces since often such phenomena lead to meltdown or to flexural failures. Such difficulties may be avoided by minimizing the functional

$$\mathcal{J}_3(T) = \int_{\Gamma_s} |T - T_s|^2 \, d\Gamma\,,$$

where T denotes the temperature, Γ_s the portion of the boundary along which one would like to avoid hot spots, and T_s a desired temperature distribution.

One of the control mechanisms that we have considered is the velocity, or mass flux, along portions of the boundary, i.e., *injection or suction of fluid*. Thus, if Γ_c denotes the portion of the boundary covered by orifices, we would seek a control $\mathbf{g}$ such that a desired objective functional is minimized, subject to the appropriate flow equations, and also such that

$$\mathbf{u} = \mathbf{g} \quad \text{on } \Gamma_c\,.$$

A second control mechanism that we have considered is *heating or cooling along bounding surfaces*. For example, one could seek a control q such that a desired objective functional is minimized, subject to the appropriate flow equations, and also such that

$$\frac{\partial T}{\partial n} = q \quad \text{on } \Gamma_c\,.$$

where Γ_c denotes the portion of the boundary along which one allows the control to act and $\partial/\partial n$ denotes the normal derivative at the boundary. A third type of control is a *distributed control*, e.g., one could try to effect control through the body force in the Navier-Stokes equation or a heat source in the energy equation. Thus, one would seek a control, defined on the flow domain Ω or on a portion of Ω, such that some functional is minimized and subject to the appropriate flow equations. Physically, one may effect such control through a magnetic field acting on an ionized fluid or electrically conducting fluid in the first case, or through radiation mechanisms or a targeted laser beam in the latter case. Recently we have begun studying, in the context of adjoint methods, *shape controls*; in this case control is effected by adjusting the shape of the flow domain. The shape of the flow domain may be changed in many ways. For example, one could use leading and/or trailing edge flaps, or movable walls, or rudders, or propeller pitch. A related problem is the *optimal design* problem. Here, we want to choose a flow domain, e.g., the exterior of an airfoil, so that some objective is achieved.

1.3. *Computational results for a cooling control problem*

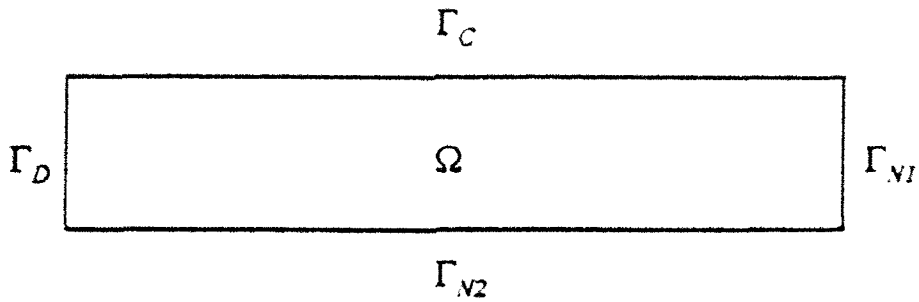
In order to illustrate the type of results that we can obtain using adjoint methods, we consider the problem of avoiding hot spots along the top wall of a rectangular channel. We assume that the flow is incompressible and convection driven so that buoyancy effects can be neglected, and thus temperature effects on the mechanical properties of the flow, i.e., the velocity and pressure, are negligible. We are interested in the design of heating and cooling controls such that hot spots are avoided along a portion of the boundary, and thus we assume that the flow is stationary. As a result of our assumptions about the flow, the state variables, i.e., the velocity $\mathbf{u}$, pressure p, and temperature T, are required to satisfy the continuity equation, the Navier-Stokes equations, and the energy equation.

In order to avoid hot spots, we minimize the functional

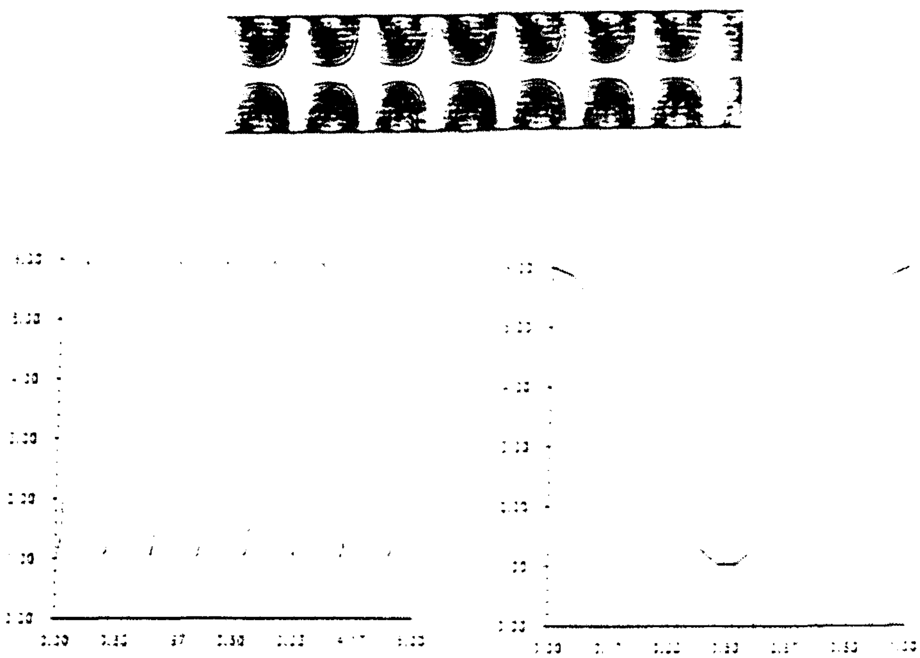
$$\mathcal{J}(T,g) = \frac{1}{2}\int_{\Gamma_s} |T - T_s|^2 \, d\Gamma + \frac{\delta}{2}\int_{\Gamma_c} |g|^2 \, d\Gamma\,, \tag{4}$$

where T is required to satisfy the flow equations along with boundary conditions. In particular, along Γ_c, the part of the boundary along which controls are allowed to act, we have that $\partial T/\partial n = g$. Γ_s denotes the part of the boundary along which we wish to match the temperature T to a desired temperature distribution T_s. The above functional has been penalized by a norm of the control; this is necessary since we are not placing any a priori constraints on the size of the control. The parameter δ is used to adjust the relative sizes of the two terms contributing to the functional.

The flow domain is the rectangular channel depicted in the accompanying figure. All computations were carried out using piecewise linear finite elements on a triangular mesh.



In the next figure we show the uncontrolled temperature in the interior as well as along the top (wall) and right (outflow) boundaries. One sees that there are many peaks along the top boundary, and that there are peaks in the temperature at the top and bottom of the outflow boundary.



Top:	level lines of the uncontrolled temperature;
Bottom-left:	uncontrolled temperature along the top wall Γ_c;
Bottom-right:	uncontro. temperature along the right (outflow) boundary Γ_{N_1}.

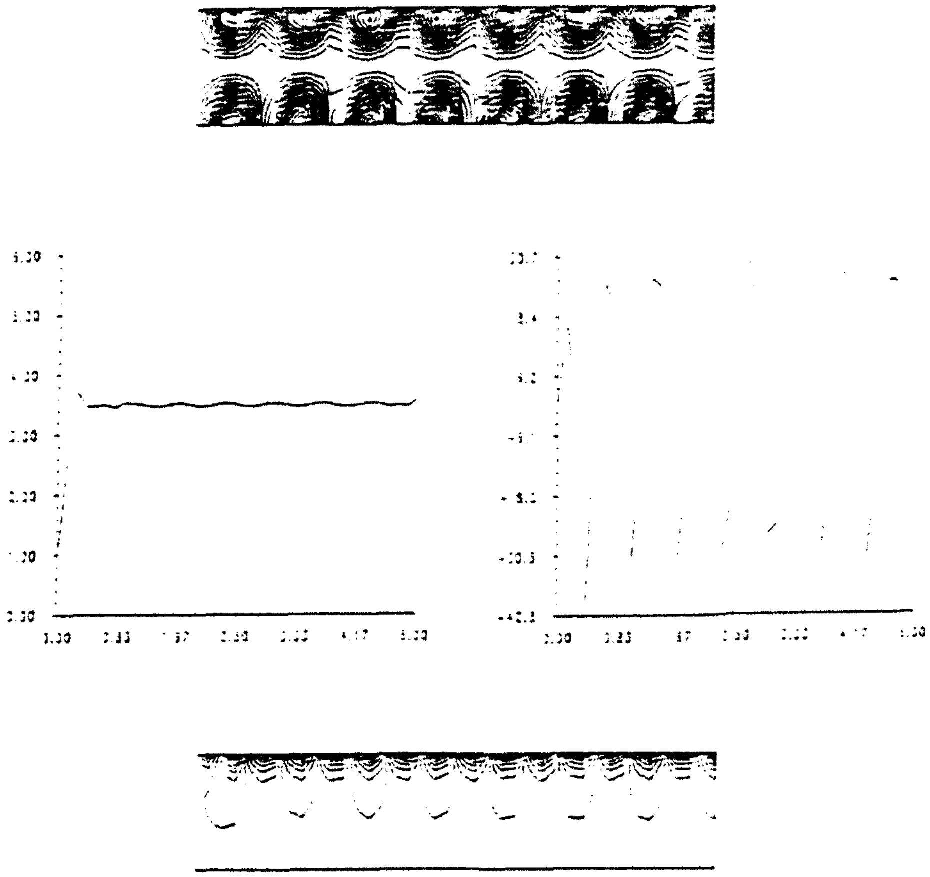
Next, we have a heat flux control acting along Γ_c, the top boundary, so that

$$\frac{\partial T}{\partial n} = g \quad \text{on } \Gamma_c ,$$

where g denotes the control. We also have that $\Gamma_s = \Gamma_c$, the top boundary, with the target temperature along Γ_s appearing in the functional (4) taken to be

$$T_s = \min\{3.5, 11.875x - 1\} \qquad \text{on } \Gamma_s = \Gamma_c . \tag{5}$$

This function ensures a continuous transition with respect to the inflow temperature which is set to $T = 1$. In the next figure we display the optimal temperature T and co-state in the interior and the optimal temperature T and control g along the top wall $\Gamma_s = \Gamma_c$. We see from the graph of T along Γ_s that we have very effectively matched the given distribution T_s given by (5). The control in this case involves both cooling and heating.

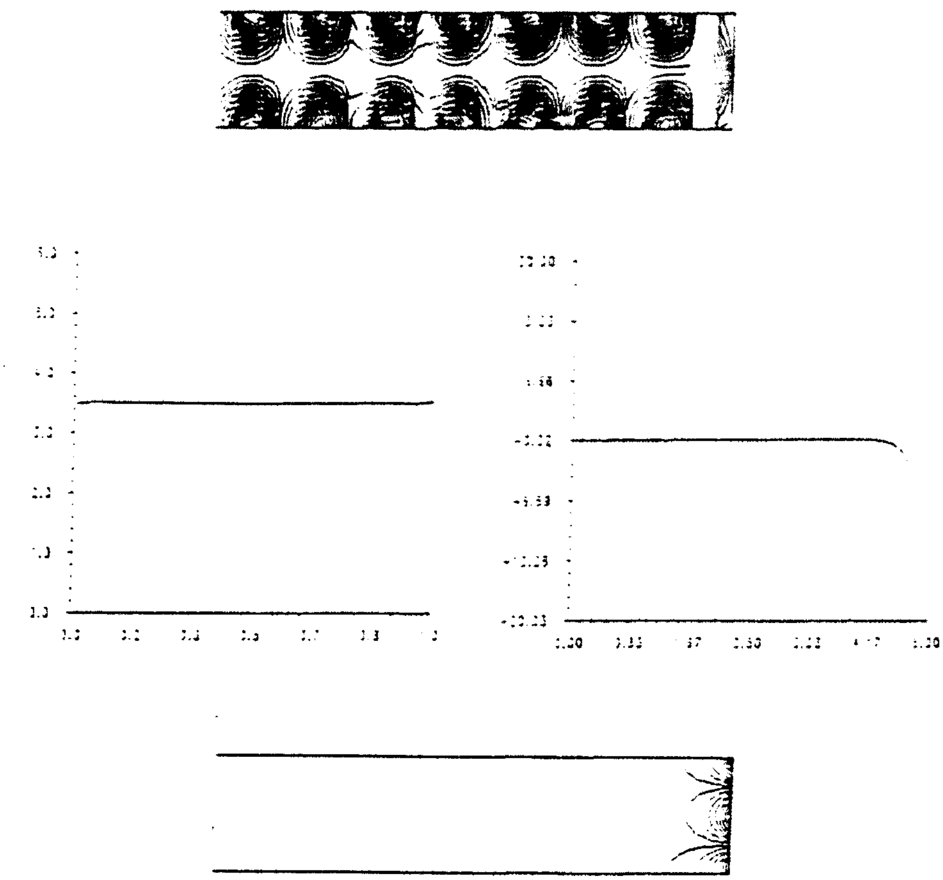


Control and target temperature on the top wall .
Top: level lines of the optimal temperature;
Left-center: optimal temperature along the top wall $\Gamma_s = \Gamma_c$;
Right-center: optimal control along the top wall Γ_c;
Bottom: level lines of the optimal co-state.

Next, we choose $\Gamma_s = \Gamma_{N1}$, the right or outflow boundary, so that $\Gamma_s \neq \Gamma_c$; we now have the target temperature

$$T_S = 3.5 \qquad \text{on } \Gamma_s = \Gamma_{N1}. \tag{6}$$

Again, in the next figure, we display the optimal temperature T and co-state in the interior, the optimal temperature T along the outflow boundary $\Gamma_s = \Gamma_{N1}$, and control g along the top wall Γ_c. Once again, an excellent job is done of matching to the prescribed temperature distribution (6). Note that the optimal control requires cooling along the top boundary only in the vicinity of the outflow boundary, i.e., near the location at which we are trying to match the flow temperature to that given by (6).



Control on the top wall Γ_c and target temperature on the right (outflow) boundary $\Gamma_s = \Gamma_{N1}$.
Top: level lines of the optimal temperature;
Left-center: optimal temperature along the outflow boundary $\Gamma_s = \Gamma_{N1}$;
Right-center: optimal control along the top wall Γ_c;
Bottom: level lines of the optimal co-state.

2. Analysis and Approximation of Macroscopic Models for Superconductivity

Superconductivity is one of the Grand Challenges identified as being crucial to future economic prosperity and scientific leadership. Much of the research in superconductivity addresses the microstructure of superconductors; one goal of that research is to predict new high critical temperature superconducting materials that may then be used in beneficial technological applications. Parallel to these efforts, it is important to study the macroscopic behavior of superconductors. Indeed, once new and usable materials are identified, their incorporation into superconducting devices depends on being able to model these devices and to numerically simulate their physical behavior. Thus, scientists, engineers, and mathematicians who wish to design superconducting devices and/or who wish to study the physics of superconductivity are in need of robust and efficient algorithms and codes for the numerical simulation of superconducting phenomena. Our goals are:

- to develop, analyze, and implement algorithms that are applicable to high-temperature superconductors; and
- to use these codes to study, in collaboration with physicists and material scientists, superconducting phenomena.

We have already passed a necessary stepping stone towards meeting these goals, namely the development and implementation of methods for low-temperature superconductors. In addition, we have obtained new analytical results in this setting. A summary of the results obtained are reported on in the papers listed in §III. Our work on superconductivity is receiving widespread recognition. We have been invited to numerous meetings and workshops on the subject, and physicists at government labs, universities, and industry have expressed interest in collaborating with us and using our algorithms. One collaborative program that has been initiated is with the group at Oxford University headed by John Ockendon.

The major accomplishments resulting from our work on low-temperature superconductivity is that our work represents the first successful simulation of superconductivity by a standard numerical technique (a finite element method); our algorithms, compared to previous efforts, are efficient, robust, and extendible to more complex settings, including some involving high critical temperature superconductors.

2.1. *Summary of theoretical results*

We summarize the theoretical aspects of our preliminary work; most details can be found in the papers on superconductivity listed in §II.

We first focused on Ginzburg-Landau models for bounded two- or three-dimensional regions representing material samples. We reviewed the mathematical formulations of some important physical concepts such as the fluxoid quantization and several important scales and parameters. Mathematically, the electromagnetic state of the superconductor corresponds to a minimizer of the Gibbs free energy which, in non-dimensionalized form, may be formulated as

$$\mathcal{G}(\psi, \mathbf{A}) = \int_\Omega \left(f_n - |\psi|^2 + \frac{1}{2}|\psi|^4 + \left| \left(\frac{i}{\kappa}\nabla + \mathbf{A} \right) \psi \right|^2 + |\mathbf{h}|^2 - 2\mathbf{h}\cdot\mathbf{H} \right) d\Omega\,, \tag{7}$$

where ψ, $\mathbf{A}$, and $\mathbf{h} = \operatorname{curl}\mathbf{A}$ denote the non-dimensionalized complex order parameter, magnetic potential, and magnetic field, respectively; $\mathbf{H}$ is the applied field. The constant f_n is the free energy density of the normal state in the absence of a magnetic field, and κ, known as the Ginzburg-Landau

parameter, is a material constant representing the ratio of penetration length to the coherence length. For type-I superconductors, we have $\kappa < 1/\sqrt{2}$, while $\kappa > 1/\sqrt{2}$ for type-II superconductors. A formal study on the transition between different states in both the type-I and type-II superconductors has also been carried out.

The Ginzburg-Landau functional (7) has a very important property, namely, that of gauge invariance. That is, if for some $\phi \in H^2(\Omega)$, the standard Sobolev space whose elements and their derivatives of order up to two are square integrable on Ω, we have

$$\zeta = \psi e^{i\kappa\phi} \quad \text{and} \quad \mathbf{Q} = \mathbf{A} + \nabla\phi\,,$$

then $(\zeta, \mathbf{Q})$ and $(\psi, \mathbf{A})$ are said to be *gauge equivalent*; note that $\mathcal{G}(\zeta, \mathbf{Q}) = \mathcal{G}(\psi, \mathbf{A})$. Based on this, the existence of minimizers of the Ginzburg-Landau functional in the space $H^1(\Omega) \times \mathbf{H}^1_n(\Omega)$ was established via standard variational arguments. (For definitions of the related spaces, we refer to the papers listed in §III.) In fact, we showed that any minimizer of the Ginzburg-Landau functional is gauge equivalent to a solution which has a divergence free magnetic potential with vanishing normal component on the boundary. This corresponds to the Coulomb gauge. The Ginzburg-Landau equations and natural boundary conditions in the Coulomb gauge are given by

$$\left(\frac{i}{\kappa}\nabla + \mathbf{A}\right)^2 \psi - \psi + |\psi|^2\psi = 0 \quad \text{in } \Omega\,, \tag{8}$$

$$\operatorname{curl}\operatorname{curl}\mathbf{A} = -\frac{i}{2\kappa}(\psi^*\nabla\psi - \psi\nabla\psi^*) - |\psi|^2\mathbf{A} + \operatorname{curl}\mathbf{H} \quad \text{in } \Omega\,, \tag{9}$$

$$\operatorname{div}\mathbf{A} = 0 \quad \text{in } \Omega \quad \text{and} \quad \mathbf{A}\cdot\mathbf{n} = 0 \quad \text{on } \Gamma\,, \tag{10}$$

and

$$\left(\frac{i}{\kappa}\nabla\psi + \mathbf{A}\psi\right)\cdot\mathbf{n} = 0 \quad \text{and} \quad \operatorname{curl}\mathbf{A}\times\mathbf{n} = \mathbf{H}\times\mathbf{n} \quad \text{on } \Gamma\,. \tag{11}$$

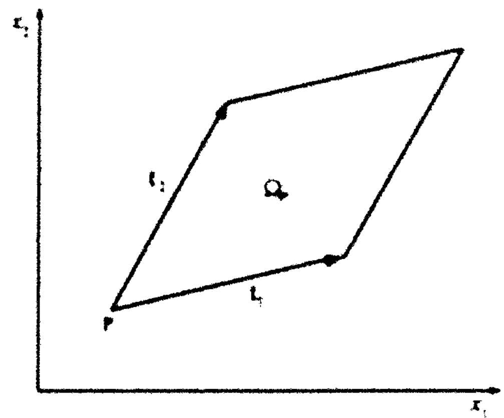
Other possible boundary conditions were also considered. Various mathematical properties of the solutions of the Ginzburg-Landau equations were studied. These included the proof of non-existence of local maxima for the Ginzburg-Landau functional and the fact that the order parameter is bounded by its ideal superconducting value, i.e., in non-dimensionalized form, $|\psi| \leq 1$ almost everywhere. Simple analytic solutions and trivial solutions were discussed. Many of the properties may be used to interpret related physical phenomena such as the perfect Meissner effect in the absence of an applied field and the existence of a mixed state, i.e., the existence of vortices or filaments, in the presence of an applied field below a critical value.

We also developed and analyzed finite element algorithms for approximating solutions to the model. Finite element subspaces are constructed, in a standard way, from partitions of Ω into finite elements; h will denote some measure of the size of the finite elements in the partition. Finite element approximations are then defined based on a weak formulation of the Ginzburg-Landau equations with the gauge $\operatorname{div}\mathbf{A} = 0$ in Ω and $\mathbf{A}\cdot\mathbf{n} = 0$ on Γ. We proved the convergence of the finite element solutions to a branch of regular solutions of the nonlinear Ginzburg-Landau equations and the convergence was shown to be uniform for κ in a compact interval. Optimal error estimates were also derived under the usual regularity assumptions. However, we note that the question of the regularity of the solutions of the Ginzburg-Landau equations in bounded domains has not been fully resolved.

While our analyses and algorithms were valid for both the type-I and type-II regimes, it is of use mostly for type-I superconductors. It is well-known that in type-II superconductors the solutions exhibit much more complicated structures. The grid size necessary to resolve the fine structures based on bounded domain models, in any computation of practical utility, would be prohibitively small. So, we turned our attention to a *periodic Ginzburg-Landau model* which, from a practical viewpoint, is more suitable for the numerical simulation of type-II superconductors.

The periodic model is based on the notion of fluxoid quantization and is formulated to describe two-dimensional thin films. The central assumption in the derivation of the model is that away from bounding surfaces, certain physical variables, such as the magnetic field, the current, and the density of superconducting charge carriers, exhibit periodic behavior with respect to a two-dimensional lattice; the accompanying figure shows a typical cell in the lattice. The non-orthogonal lattice is not necessarily aligned with the coordinate axes (consult the figure). A function f is *periodic with respect to the lattice vectors* $\mathbf{t}_1$ *and* $\mathbf{t}_2$ if

$$f(\mathbf{x} + \mathbf{t}_k) = f(\mathbf{x}) \qquad \text{for } k = 1, 2 \text{ and } \forall\, \mathbf{x} \in \mathbb{R}^2 \tag{12}$$



The cell Ω_P determined by the lattice vectors $\mathbf{t}_1$ and $\mathbf{t}_2$ and the point $\mathbf{P}$

We were first concerned with the formulation of the model. A very important issue is the choice of gauge. A gauge choice is constrained by the need to enforce the periodicity of several physical variables and by the fluxoid quantization condition; it is made more difficult by the fact that these constraints result in nonstandard "quasi"-periodic conditions for the primary variables in the Ginzburg-Landau model, i.e., the order parameter and magnetic potential. There have been conflicting discussions related to this issue in the literature. We made a rigorous and detailed study and were able to define consistent gauge choices. In short, given the lattice cell depicted in the above figure, we showed that the vector magnetic potential is gauge equivalent to a potential of the form $\mathbf{Q} - \mathbf{A}_0$ where

$$\mathbf{A}_0 = \frac{\bar{B}}{2}\begin{pmatrix} x_2 \\ -x_1 \end{pmatrix} \tag{13}$$

and $\mathbf{Q}$ is divergence free, periodic, and is uniquely determined up to an additive constant vector. In (13), $\bar{B}$ is the average magnetic field. To maintain the periodicity of the desired physical variables,

the order parameter should satisfy

$$\zeta(\mathbf{x} + \mathbf{t}_k) = \zeta(\mathbf{x}) e^{i\kappa g_k(\mathbf{x})} \quad \forall\, \mathbf{x} \in \Gamma_{-k},\ k = 1, 2, \tag{14}$$

where $g_k(\mathbf{x}) = -\bar{B}(\mathbf{x} \times \mathbf{t}_k)/2$, $k = 1, 2$, and where Γ_{-1} and Γ_{-2} denote the left and bottom edges of the lattice cell, respectively. Clearly, (14) implies the periodicity of the magnitude of the order parameter; however, the phase suffers a jump across the lattice. The fluxoid quantization condition holds under this gauge choice.

We discussed the equivalence of the different forms of the Ginzburg-Landau functional in the periodic setting and proved the existence of the minimizer in the appropriate spaces. Minimizers satisfy a system of equations similar to (8) and (9), with suitable modifications to the boundary conditions. Then, we derived various properties of the solutions of the Ginzburg-Landau equations. Some of the results, such as the boundedness of the order parameters and the discussion on simple analytic solutions, are similar to those we obtained for the bounded domain case. Unlike that case for which the study of the regularity of solutions was limited, we were able to obtain extensive regularity results for the periodic problem.

We then considered finite element approximations of solutions of the periodic model. Periodic models have been used in the past as a setting for analyzing and approximating phenomena in type-II superconductors using for the most part, some type of series solution or a Monte Carlo/simulated annealing approach. As in other settings, finite element methods can be very competitive for numerical simulation purposes.

Basically, we employ the standard Galerkin finite element approximation to solve the nonlinear Ginzburg-Landau equations. The periodicity of the physical variables and boundary conditions such as (14) for the primary variables are the non-standard features of our scheme. In general, functions in the finite element space only satisfy (14) at the interpolating nodes on the boundary, i.e.,

$$\zeta^h(\mathbf{x}_j + \mathbf{t}_k) = \zeta^h(\mathbf{x}_j) e^{i\kappa g_k(\mathbf{x}_j)} \quad \forall\, \mathbf{x}_j \in \Gamma_{-k},\ k = 1, 2, \tag{15}$$

where $\mathbf{x}_j$ is any boundary vertex of a triangle for piecewise linear and quadratic elements and it may also be the midpoint of any triangle edge on the boundary for quadratic elements. The periodicity of finite element solutions with respect to the lattice is also defined only at interpolating nodes. Thus, the finite element spaces are not the subspaces of the exact solution spaces. The study of the approximations centered around this issue.

The key to the error analysis is an estimate of a boundary integral term which would disappear if the finite element spaces were subspaces of the underlying solution space for the continuous problem. We showed that this integral, although not zero in general, gives a higher order error term in the final estimate and therefore, the optimal convergence rates are retained. The idea may well be generalized to higher order element cases with suitable choices of interpolation procedures. Thus, we were able to obtain optimal error estimates for approximations to the solution of the full nonlinear, periodic, Ginzburg-Landau equations.

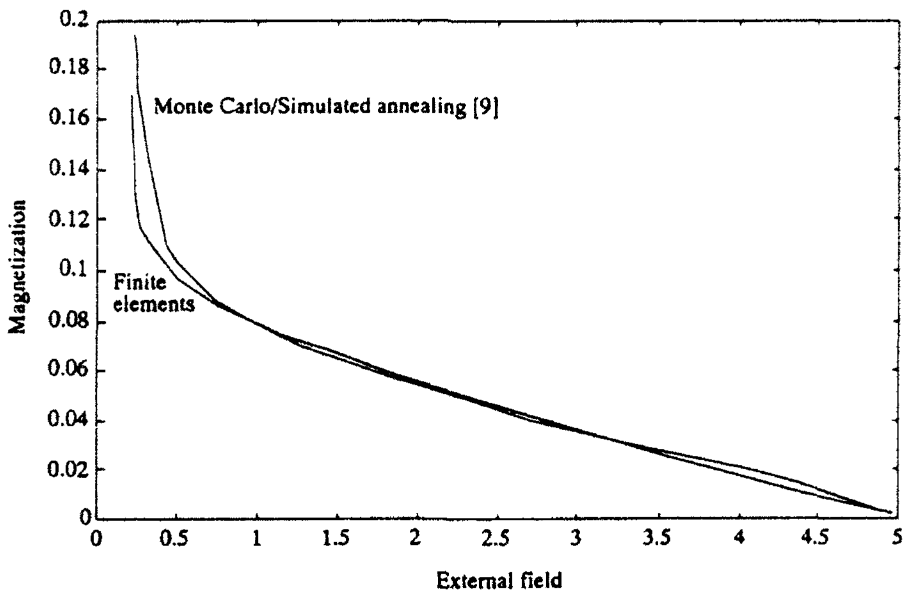
2.2. *Summary of computational results*

We have developed a finite element code for the periodic Ginzburg-Landau model discussed above. The code uses piecewise quadratic finite element functions based on a triangulation of a lattice cell. The periodicity and "quasi"-periodicity conditions are implemented as described by

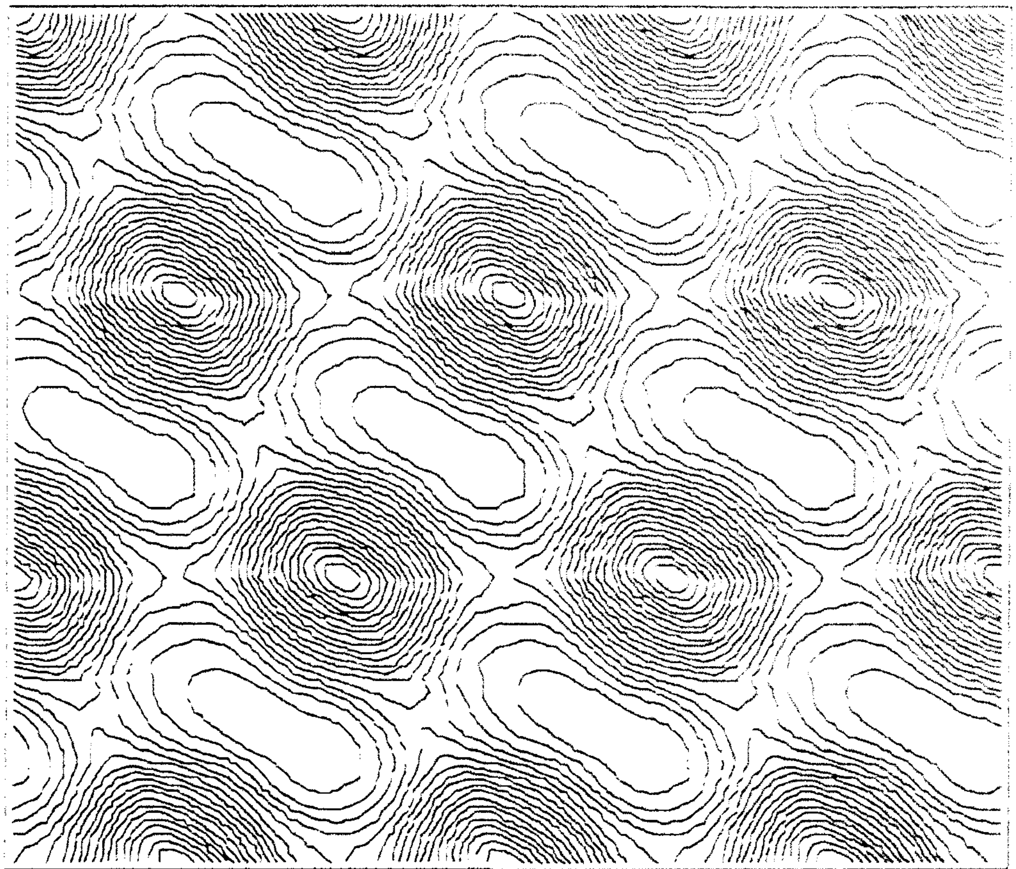
(15), i.e., at the nodes of the finite elements. The most interesting periodicity structure is that of an equilateral triangular lattice having one fluxoid associated with each lattice cell. Indeed, it is well-known that such a lattice yields the smallest value for the Gibbs free energy. Having chosen input data corresponding to an equilateral triangular lattice having one fluxoid associated with each lattice cell, the only remaining inputs to be chosen are the Ginzburg-Landau parameter κ, the average magnetic field $\bar{B}$, and the number and spacing of the grid lines.

The discretized equations are a nonlinear system of algebraic equations. These are solved by a continuation method coupled with Newton's method. The code is configured so that one chooses a fixed value for κ, and then varies $\bar{B}$. For each pair $(\kappa, \bar{B})$, Newton's method is used to solve the nonlinear equations. The initial guess for Newton's method is determined by continuing from the solution determined for a previous value of $\bar{B}$ and the same value of κ. The particular continuation method used is a tangent line approximation to the solution at the previous value of $\bar{B}$. We start with a value of $\bar{B}$ close to the upper limit κ for which Newton's method seems to have a large attraction ball; we then continue by successively reducing the value of $\bar{B}$ towards its lower limit 0.

The graph of the computed approximation of the magnetization $-4\pi M$ vs. the applied field H_e and the level curves of the density of superconducting electrons N, are given in the next two figures, respectively. These results were obtained on a Macintosh II using 3 uniformly spaced intervals in each of the lattice directions. For comparison purposes, we also provide, in the first figure, the corresponding graph for a Monte Carlo/simulated annealing approximation. For the second figure, the solution in only a single lattice cell was computed; this solution was extended, using periodicity or "quasi"-periodicity relations to obtain the solution outside the computational cell.



Comparison of computational results for the magnetization $(-4\pi M)$ vs. external field (H_e) for $\kappa = 5$.



Level curves of N_s, the density of superconducting charge carriers, for $\kappa = 5$ and $\bar{B} = 10/3$.

II - SUMMARY OF OTHER RESEARCH PROJECTS

Under the sponsorship of AFOSR Grant Number AFOSR-90-0179, we have also engaged in a number of other research projects. Here we give brief descriptions of some of our accomplishments. Details may be found in the papers listed in §III.

- *Parallel algorithms for flow calculations based on the velocity-vorticity formulation.* We carried out a careful study of the accuracy of the approximations of the Navier-Stokes through the use of the velocity-vorticity formulation. We have shonw that most of the existing boundary treatments lead to bad vorticity approximations, and we have also developed improved treatments. We have demonstrated how this formulation can be used to advantage in a parallel computing envirnment. Specifically, for methods of solution of the Navier-Stokes equations that require the solution of a series of Stokes problems, we have shown how the latter may be solved as a sequence of uncoupled Poisson problems. Thus we have coarse-grain parallelism; fine-grain parallelism may also be attained within each of the Poisson solves.
- *Analysis, application, and computation of centroidal Voronoi tesselations.* Voronoi tesselations, and their dual Delauny tesselations of great use in a variety of seetings, including numerical analysis, data compression, etc. We examine the special type of Voronoi tessela-

tion wherein the points from which the Voronoi regions are defined are also the centroids of those regions. We have shown that this type of tesselation possess a certain optimality property that makes them useful in applications. We have also analyzed algorithms for the determination of such tesselations.

- *The treatment of inhomogeneous essential boundary conditions and the accurate computation of stresses along boundaries in the finite element method.* The "basic" finite element method applies to homogeneous Dirichlet boundary conditions. A variety of treatments of inhomogeneous boundary conditions has been proposed in the literature. In our work, we studied the most popular treatment in engineering practice, namely approximating the inhomogeous data by a boundary interpolant. We also studied Lagrange multiplier methods, and, in particular, developed a class of specific methods that are optimally accurate and for which the Lagrange multiplier computation uncouples. We made a comprehensive, rigorous study of the accuracy of these various treatments. As a side benefit, we devised an algorithm for the accurate calculation of boundary stresses in fluid flow calculations. We also analyzed the accuracy of these stress approximations.

III - SUMMARY OF OTHER ACTIVITIES UNDER GRANT AFOSR-90-0179

Book editing project

- Editing a book (with R.A. Nicolaides) to be published by Cambridge University Press on recent trends and advances in incompressible flow calculations.

Personnel supported by the grant

- Max Gunzburger (Principal investigator) - Summer salary.
- Jerome Eastham (Visiting Assistant Professor) - Partial academic year salary.
- Mark Mundt (Ph.D. student) - Academic year salary.
- Pavel Bochev (Ph.D. student) - Summer salary.
- H. Lee (Ph.D. student) - Summer salary.
- John Burkhardt (Ph.D. student) - Academic year and summer salary.

Conferences, workshops, and special sessions organized on grant related research

- Special Session on Control of Partial Differential Equations, World Congress of Nonlinear Analysts, Tampa, August, 1992, (with J. Burns and T. Herdman).
- Workshop on Flow Control, IMA, Minneapolis, November, 1992.
- Special Session on Flow Control, IEEE Conference on Decision and Control, Tuscon, December, 1992, (with K. Ito).
- AMS-SIAM-IMS Summer Research Conference on Superconductivity, site to be announced, July, 1993, (with J. Ockendon).

Invited talks in 1991-1992 on grant related research

- International Conference on Differential Equation, Edinburg, TX, May, 1991.
- Seventh International Conference on Numerical Methods in Laminar and Turbulent Flow, Stanford, July, 1991.
- Second Soviet-North American Workshop on Computational Fluid Dynamics, Montreal, September, 1991.
- Fourth International Symposium on Computational Fluid Dynamics, Davis, CA, September, 1991.
- Workshop on Superconductivity, Argonne, IL, January, 1992.
- The Mathematics of Superconductivity, Edinburgh, Scotland, January, 1992.
- Joint Meeting of the American and London Mathematical Societies, Cambridge, England, June, 1992.
- World Congress of Nonlinear Analysts, Tampa, August, 1992.

- Computation and Control III, Bozeman, MT, August, 1992.
- Sixth International Conference on Boundary and Interior Layers, Summit Country, CO, August, 1992.
- Conference on Computational Methods for the Material Sciences, Pittsburgh, September, 1992.
- American Mathematical Society Meeting, Dayton, October, 1992.
- IEEE Conference on Decision and Control, Tuscon, December, 1992.

Publications prepared reporting on grant related research (1990-1992)

1. Finite element approximations of a Ladyzhenskaya model for stationary incompressible viscous flow; *SIAM J. Numer. Anal.* **27**, 1990, 1-19; with Q. Du.
2. Experiences with computational methods for the velocity-vorticity formulation of incompressible viscous flow; *Computational Methods in Viscous Aerodynamics*, Elsevier, 1990, 231-271; with M. Mundt and J. Peterson.
3. A subdomain Galerkin/least squares method for first order elliptic systems in the plane; *SIAM J. Numer. Anal.* **27**, 1990, 1197-1211; with C. Chang.
4. A numerical method for drag minimization via the suction and injection of mass through the boundary; *Stabilization of Flexible Structures*, Springer, 1990, 312-321; with L. Hou and T. Svobodny.
5. Finite element approximations of an optimal control problem associated with the scalar Ginzburg-Landau equation; *Comput. Math. Appl.* **21**, 1991, 123-131; with L. Hou and T. Svobodny.
6. Analysis of a Ladyzhenskaya model for incompressible viscous flow; *J. Math. Anal. Appl.* **155**, 1991, 21-45; with Q. Du.
7. Analysis, approximation, and computation of control problems for incompressibe flows; *Turbulence Structure and Control*, Ohio State, 1991, 85-88.
8. Existence, uniqueness, and finite element approximation of solutions of the equations of stationary, incompressible magnetohydrodynamics; *Math. Comp.* **56**, 1991, 523-563; with A. Meir and J. Peterson.
9. Control of temperature distributions along boundaries of engine components; *Numerical Methods in Laminar and Turbulent Flow* VII, Pineridge, 1991, 765-773; with L. Hou and T. Svobodny.
10. Vorticity constraints in velocity-vorticity formulations of steady, viscous, incompressible flow; *Numerical Methods in Laminar and Turbulent Flow* VII, Pineridge, 1991, 774-781; with Q. Du and A. Meir.
11. Approximation of boundary control and optimization problems for fluid flows; *4th International Symposium on Computational Fluid Dynamics*, U. California, Davis, 1991, 455-460; with L. Hou and T. Svobodny.
12. Analysis and finite element approximations of optimal control problems for the stationary Navier-Stokes equations with distributed and Neumann controls; *Math. Comp.* **57** 1991, 123-151; with L. Hou and T. Svobodny.
13. Predictor and steplength selection in continuation methods for the Navier-Stokes equations; *Comput. Math. Appl.* **22**, 1991, 73-81; with J. Peterson.
14. Analysis and finite element approximations of optimal control problems for the stationary Navier-Stokes equations with Dirichlet controls; *Math. Model. Numer. Anal.* mbf 25, 1991, 711-748; with L. Hou and T. Svobodny.
15. Boundary velocity control of incompressible flow with an application to viscous drag reduction; *SIAM J. Control Optim.* **30** 1992, 167-181; with L. Hou and T. Svobodny.
16. Analysis and approximation of the Ginzburg-Landau model of superconductivity; *SIAM Review* **34** 1992, 54-81; with Q. Du and J. Peterson.
17. Numerical solution of the compressible boundary layer equations using the finite element method; AIAA Paper AIAA-92-0666, AIAA, Washington, 1992; with E. Hytopoulos and J. Schetz.

18. Treating inhomogeneous essential boundary conditions in finite element methods and the calculation of boundary stresses; *SIAM J. Numer. Anal.* **29** 1992, 390-424; with L. Hou.
19. Solving the Ginzburg-Landau equations by finite element methods; *Phys. Rev. B*; **46** 1992, 9027-9034; with Q. Du and J. Peterson.
20. On the Ginzburg-Landau equations of superconductivity; *Partial Differential Equations*, Longman, 1992, 58-62; with Q. Du and J. Peterson.
21. Heating and cooling control of temperature distributions along boundaries of flow domains; to appear in *J. Math. Systems Estim. Control*; with L. Hou and T. Svobodny.
22. Optimal control and optimization of viscous, incompressible flows; to appear in *Incompressible Computational Fluid Dynamics: Trends and Advances*; with L. Hou and T. Svobodny.
23. Boundary control of incompressible flows; to appear in *Advances in Computational Fluid Dynamics*; with L. Hou and T. Svobodny.
24. Modeling and analysis of a periodic Ginzburg-Landau model for type-II superconductors; to appear; with Q. Du and J. Peterson.
25. Optimal control problems for a class of nonlinear equations with an application to the control of fluids; to appear; with L. Hou and T. Svobodny.
26. Finite element approximation of a periodic Ginzburg-Landau model for type-II superconductors; to appear; with Q. Du and J. Peterson.
27. The approximation of boundary control problems for fluid flows with an application to control by heating and cooling; to appear; with L. Hou and T. Svobodny.
28. Analysis, applications, and computation of centroidal Voronoi tesselations; in preparation; with Q. Du, V. Faber, and C. Scovill.